Fuels/Chemicals from Syngas Breakout

Model Development Issues

Participants:
Edward Brandner
Santosh Gangwal
James Tilton
Dragomir Bukur
Lynn Layman
Jack Halow
Issac Gamwo
Madhava Syamlal
Jerry Boyle

Models needed for:
A) Separation devices (Fe catalyst/wax)
B) Slurry bubble column reactor (SBCR)
C) Wax upgrading reactor
D) Reliability & safety

1. Technology Module Barriers:
A) Catalyst deactivation and aging (fouling, poisoning, sintering)
B) Kinetic rate data and model
C) Catalyst selectivity
D) Catalyst/wax separation and catalyst attrition
E) Uncertainty in hydrodynamic scale-up
F) Feedstock and product mix flexibility
G) Inadequate knowledge of physical properties and phase equilibrium
H) Absence of a well validated SBCR model

Most important design and control models.
Erosion is not much of a problem

2. Model Priority:
- Fe catalyst aging behavior
- SBCR

3. Model usage, provide guidance to technology developers:
A) Catalyst replacement rate including cost
B) Design and optimization of catalyst and reactor

Speed vs. Accuracy, increasing capital costs are pushing smaller margins of error:
A) In equipment design stage of important component, 1 week
B) Design of less important components, instantaneous

C) Plant simulations, 1 minute
D) Control, real time
E) Equipment size accuracy +/- 20%
F) Temperature better than 10% accuracy

4) Barriers to Model Development:
A) Slurry Bubble Column Reactor:
Need experimental data on at least 4"
B) Catalyst aging
Develop a accelerated aging test (e.g. simulate 3 years operation is 3 weeks)
C) General
Validation of the computational model using scale-up data
Fast computers (e.g. to test grid independence of the results)
Need better constitutive models

Strategies:
A) Establish consortium for attacking specific problems
B) Establish challenge problems (e.g. experimental testing and synthetic problem)

5. State-of-Art Models:
A) IIT/NETL code for slurry bubble column
B) Dudokovic at Washington University based on CFDLIB (from LANL)
C) Krishna University of Amsterdam based on CFX
D) L-S Fan U of Ohio
E) Flow sheet models: ASPEN+, Hysys
F) CFD packages: Fluent, CFX
G) CAD: ProE, Ansys, Autocad, Intergraph

6) Importance to Technology Developers
A) Economic/risk, cfd codes, process engineering, control, CAD, integration/portability
B) Internet based concurrent engineering, immersive visualization

Information Exchange & Communication
Communication Issues:
A) Survey modeling needs of technology developers
B) Publicly available models of components (performance and cost)
C) Better information exchange between experimentalist and modelers
D) Better information exchange among modelers
E) Intellectual property concerns hinder communication

1. Plans for information exchange (Who will fund efforts?):
A) Smaller work groups with government, academia and industry
B) On DOE projects force teams to include both modelers and developers
C) Have Round Robin testing of models and experiments

2. Intellectual Property Concerns:
A) Resolve IP issues upfront within consortium

Government Role
1. Software needs:
A) RFP requires every technology developer provide model of that technology
B) Models for catalyst design and SBCR

2. Balance Between New vs. Old:
A) Fund basic science and encapsulate them in constitutive laws
B) Leave rigorous numerical algorithm development to industry

3. Near/Long Term & High/Low Risk Efforts?
A) Fund long term and high risk:
B) High Risk/Near Term (7 year) Slurry Bubble Column Reactor Model, Fe catalyst model
C) High Risk/Long Term (20 year): Membrane separation model
D) High Risk/Long Term: Syngas to hydrogen models (model for chemistry & S tolerant catalyst)